



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:02 PM UTC

PDB ID : 1B3L / pdb_00001b3l
Title : OLIGO-PEPTIDE BINDING PROTEIN (OPPA) COMPLEXED WITH KGK
Authors : Tame, J.R.H.; Wilkinson, A.J.
Deposited on : 1998-12-14
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

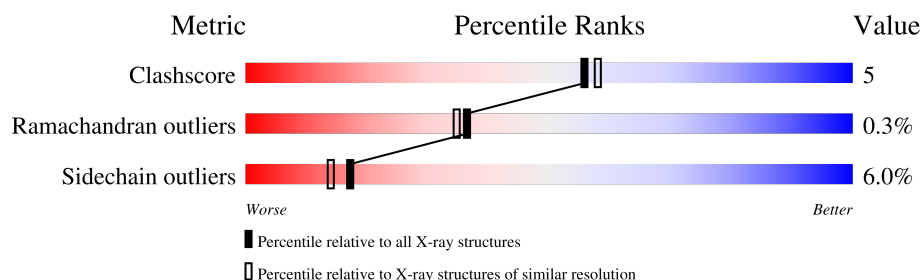
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	517	 69% 26% . .
1	C	517	 80% 17% .
2	B	3	 100%
2	D	3	 67% 33%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8730 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

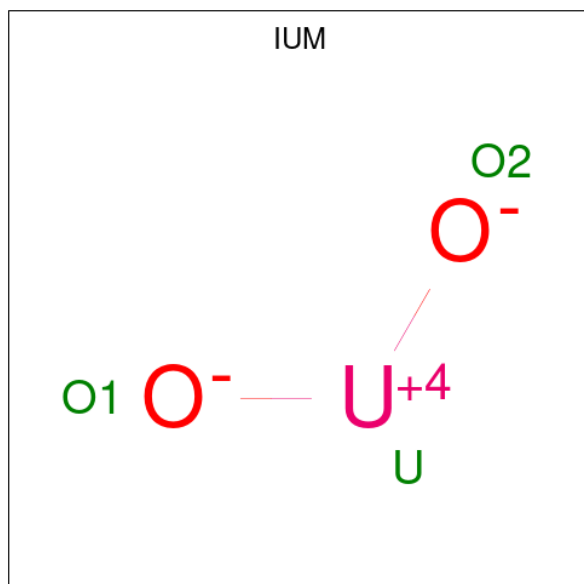
- Molecule 1 is a protein called PROTEIN (OLIGO-PEPTIDE BINDING PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	11	2	0
			4171	2671	700	795	5			
1	C	517	Total	C	N	O	S	8	4	0
			4173	2671	700	797	5			

- Molecule 2 is a protein called PROTEIN (LYS-GLY-LYS).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			23	14	5	4			
2	D	3	Total	C	N	O	0	0	0
			23	14	5	4			

- Molecule 3 is URANYL (VI) ION (CCD ID: IUM) (formula: O₂U).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total U 1 1	0	0

- Molecule 4 is water.

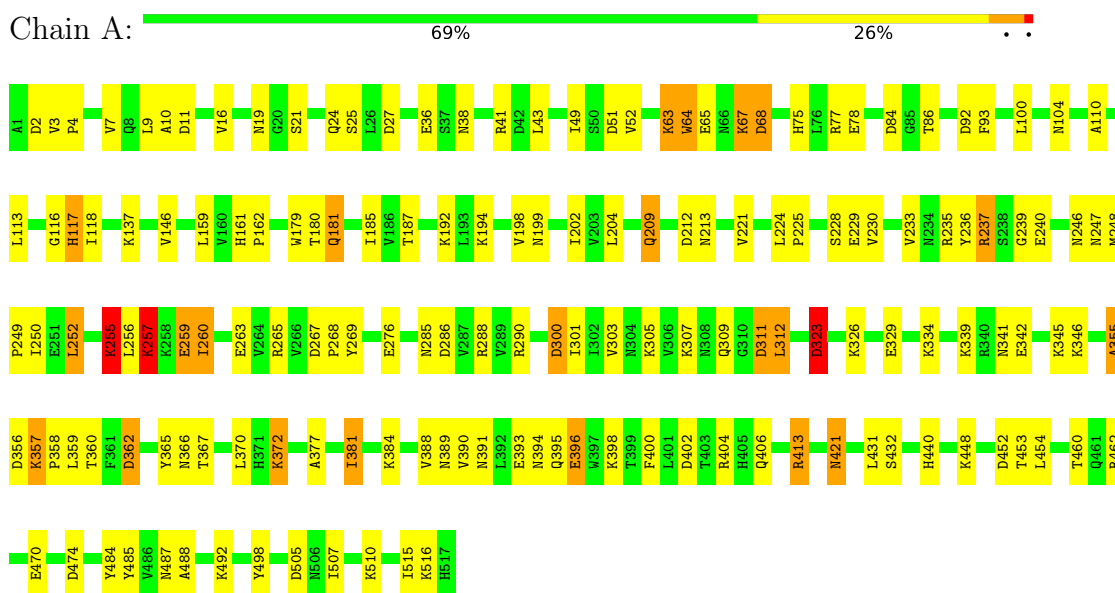
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	124	Total O 124 124	0	0
4	B	3	Total O 3 3	0	0
4	C	209	Total O 209 209	0	0
4	D	3	Total O 3 3	0	0

3 Residue-property plots

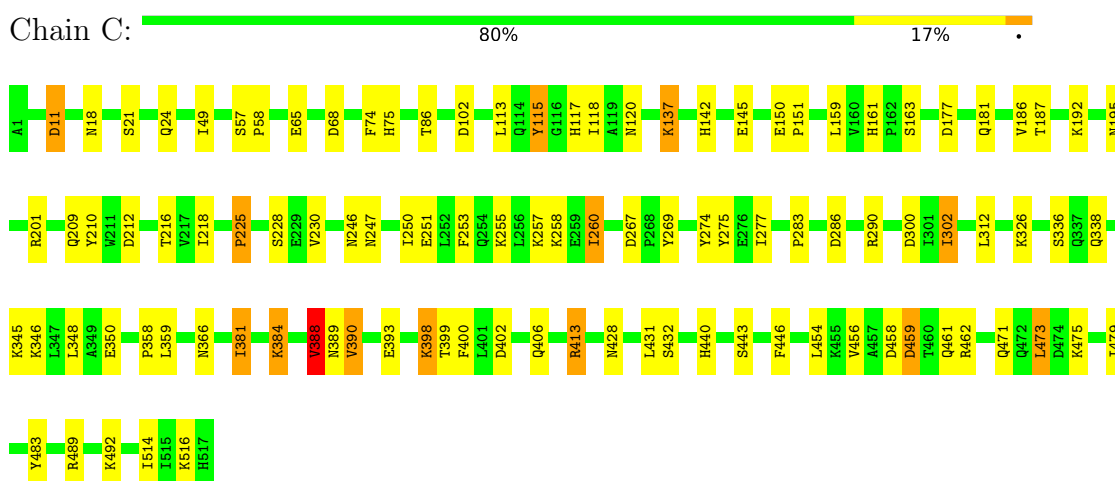
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: PROTEIN (OLIGO-PEPTIDE BINDING PROTEIN)



• Molecule 1: PROTEIN (OLIGO-PEPTIDE BINDING PROTEIN)



• Molecule 2: PROTEIN (LYS-GLY-LYS)

Chain B:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: PROTEIN (LYS-GLY-LYS)

Chain D:  67% 33%

 L1 L2 L3

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.91 Å 74.80 Å 103.77 Å 90.00° 91.10° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00	Depositor
% Data completeness (in resolution range)	94.8 (15.00-2.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.178 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8730	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IUM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.09	5/4290 (0.1%)	1.83	83/5849 (1.4%)
1	C	1.17	1/4301 (0.0%)	1.83	88/5864 (1.5%)
2	B	1.02	0/22	1.56	0/24
2	D	1.70	0/22	2.11	0/24
All	All	1.13	6/8635 (0.1%)	1.83	171/11761 (1.5%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	396	GLU	CG-CD	35.52	2.40	1.52
1	C	192	LYS	CD-CE	15.81	1.99	1.52
1	A	339	LYS	CD-CE	12.29	1.89	1.52
1	A	194	LYS	CD-CE	-8.72	1.26	1.52
1	A	192	LYS	CG-CD	5.83	1.70	1.52
1	A	116	GLY	N-CA	5.15	1.52	1.45

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	GLU	CB-CG-CD	-26.71	67.20	112.60
1	A	194	LYS	CG-CD-CE	14.21	143.99	111.30
1	C	446	PHE	CA-C-O	-12.63	107.56	120.82
1	A	259	GLU	N-CA-C	-10.11	99.07	111.40
1	A	339	LYS	CD-CE-NZ	-9.86	80.34	111.90
1	A	300	ASP	CA-CB-CG	-8.95	103.65	112.60
1	A	400	PHE	CA-CB-CG	8.94	122.74	113.80
1	C	201	ARG	CD-NE-CZ	8.79	136.71	124.40
1	A	355	ALA	N-CA-C	-8.30	99.58	110.53
1	C	192	LYS	CG-CD-CE	-8.01	92.87	111.30
1	C	117	HIS	CA-CB-CG	-7.90	105.90	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	177	ASP	CA-CB-CG	7.86	120.46	112.60
1	C	446	PHE	O-C-N	7.78	130.08	122.07
1	A	240	GLU	N-CA-C	7.74	122.41	113.19
1	C	250	ILE	CA-C-N	7.62	130.82	120.38
1	C	250	ILE	C-N-CA	7.62	130.82	120.38
1	C	432[A]	SER	CA-C-O	-7.60	112.49	120.55
1	C	432[B]	SER	CA-C-O	-7.60	112.49	120.55
1	C	458	ASP	CA-CB-CG	7.58	120.18	112.60
1	C	461	GLN	CA-CB-CG	7.55	129.21	114.10
1	C	102	ASP	CA-C-O	7.52	126.82	119.75
1	A	488	ALA	CA-C-O	7.50	128.19	120.24
1	A	235	ARG	N-CA-C	-7.48	103.99	113.72
1	A	100	LEU	O-C-N	-7.45	114.23	122.12
1	A	413	ARG	NE-CZ-NH2	-7.43	112.51	119.20
1	C	492	LYS	CG-CD-CE	7.40	128.33	111.30
1	C	443	SER	CA-C-O	7.39	125.35	119.59
1	A	104	ASN	CA-CB-CG	-7.32	105.28	112.60
1	A	255	LYS	CA-CB-CG	7.30	128.70	114.10
1	A	339	LYS	CG-CD-CE	-7.23	94.67	111.30
1	A	41	ARG	CD-NE-CZ	7.15	134.41	124.40
1	C	74	PHE	CA-CB-CG	-7.04	106.76	113.80
1	A	470	GLU	O-C-N	-7.03	114.67	122.12
1	A	288	ARG	NE-CZ-NH2	7.00	125.50	119.20
1	C	18	ASN	CA-CB-CG	-6.94	105.66	112.60
1	A	362	ASP	CA-CB-CG	-6.88	105.72	112.60
1	A	290	ARG	NE-CZ-NH2	6.87	125.39	119.20
1	A	192	LYS	CB-CG-CD	-6.75	95.78	111.30
1	C	413	ARG	NE-CZ-NH2	-6.74	113.13	119.20
1	A	285	ASN	OD1-CG-ND2	-6.72	115.88	122.60
1	A	25	SER	O-C-N	6.63	129.49	123.26
1	A	247	ASN	CA-CB-CG	6.60	119.20	112.60
1	C	300	ASP	CA-CB-CG	-6.57	106.03	112.60
1	C	366	ASN	OD1-CG-ND2	-6.57	116.03	122.60
1	A	159	LEU	N-CA-C	6.53	120.85	113.01
1	A	68	ASP	CA-CB-CG	6.53	119.13	112.60
1	C	479	ILE	CA-C-O	-6.47	115.29	121.64
1	C	400	PHE	CA-CB-CG	6.47	120.27	113.80
1	C	115	TYR	CA-C-O	-6.44	113.73	120.55
1	C	290	ARG	NE-CZ-NH2	6.36	124.93	119.20
1	C	459	ASP	CA-CB-CG	-6.34	106.26	112.60
1	A	250	ILE	CA-C-N	6.26	128.99	120.54
1	A	250	ILE	C-N-CA	6.26	128.99	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	358	PRO	N-CA-C	6.25	121.08	111.57
1	A	474	ASP	CA-C-O	6.22	127.02	120.42
1	C	440	HIS	CA-CB-CG	-6.21	107.59	113.80
1	A	311	ASP	CA-C-O	-6.21	114.67	121.87
1	A	507	ILE	CA-C-N	-6.21	114.24	122.99
1	A	507	ILE	C-N-CA	-6.21	114.24	122.99
1	C	489	ARG	CD-NE-CZ	6.19	133.07	124.40
1	A	100	LEU	CA-C-O	6.16	127.08	120.55
1	A	146	VAL	N-CA-C	6.12	116.68	107.75
1	A	440	HIS	CA-CB-CG	-6.11	107.69	113.80
1	C	102	ASP	O-C-N	-6.09	115.88	121.30
1	C	471	GLN	O-C-N	-6.09	115.67	122.12
1	A	93	PHE	CA-CB-CG	-6.08	107.72	113.80
1	A	311	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	246	ASN	CA-C-N	6.01	131.49	122.47
1	A	246	ASN	C-N-CA	6.01	131.49	122.47
1	A	64	TRP	CA-C-O	-5.99	115.04	121.45
1	C	413	ARG	CG-CD-NE	-5.98	98.85	112.00
1	A	413	ARG	NH1-CZ-NH2	5.94	127.02	119.30
1	A	303	VAL	N-CA-C	5.90	116.54	110.82
1	C	11	ASP	CA-CB-CG	-5.89	106.71	112.60
1	C	228	SER	O-C-N	-5.88	115.87	122.93
1	C	473	LEU	CA-C-O	5.87	126.77	120.55
1	C	137	LYS	CA-C-N	-5.86	114.63	122.42
1	C	137	LYS	C-N-CA	-5.86	114.63	122.42
1	A	432[A]	SER	CA-C-O	-5.84	113.50	120.10
1	A	432[B]	SER	CA-C-O	-5.84	113.50	120.10
1	A	117	HIS	CA-CB-CG	-5.83	107.97	113.80
1	A	346	LYS	CB-CG-CD	5.82	124.69	111.30
1	A	239	GLY	N-CA-C	5.80	126.92	113.18
1	C	381	ILE	O-C-N	-5.78	116.25	121.91
1	C	413	ARG	NH1-CZ-NH2	5.76	126.79	119.30
1	C	275	TYR	CA-C-O	5.76	126.52	120.36
1	C	247	ASN	CA-C-O	-5.75	114.14	120.24
1	C	68	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	290	ARG	NE-CZ-NH1	-5.74	115.76	121.50
1	A	323	ASP	CB-CA-C	-5.74	102.09	110.06
1	C	277	ILE	CA-C-O	-5.71	114.21	120.84
1	C	137	LYS	O-C-N	5.70	129.87	123.48
1	C	384	LYS	CB-CA-C	-5.70	101.94	110.88
1	C	302	ILE	N-CA-C	5.68	115.88	110.42
1	C	163[A]	SER	CA-C-O	-5.67	112.63	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	163[B]	SER	CA-C-O	-5.67	112.63	119.49
1	C	230	VAL	CA-C-O	-5.66	114.76	121.05
1	C	483	TYR	CA-CB-CG	5.66	124.09	113.90
1	A	505	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	235	ARG	CB-CA-C	5.61	118.97	109.55
1	C	274	TYR	CA-C-N	-5.60	115.32	122.77
1	C	274	TYR	C-N-CA	-5.60	115.32	122.77
1	A	286	ASP	CA-CB-CG	5.60	118.20	112.60
1	C	159	LEU	N-CA-C	5.58	119.83	113.19
1	A	75	HIS	CA-CB-CG	-5.58	108.22	113.80
1	C	120	ASN	OD1-CG-ND2	5.57	128.17	122.60
1	A	213	ASN	OD1-CG-ND2	-5.55	117.05	122.60
1	C	479	ILE	O-C-N	5.51	129.07	122.95
1	A	92	ASP	CA-CB-CG	-5.47	107.13	112.60
1	C	186	VAL	CA-C-O	-5.43	114.61	120.36
1	C	225	PRO	CA-C-N	-5.40	114.25	121.80
1	C	225	PRO	C-N-CA	-5.40	114.25	121.80
1	C	456	VAL	CB-CA-C	-5.39	105.66	111.59
1	A	181	GLN	CA-C-N	5.38	125.05	119.56
1	A	181	GLN	C-N-CA	5.38	125.05	119.56
1	C	286	ASP	O-C-N	-5.36	117.11	123.22
1	A	276	GLU	CB-CG-CD	-5.35	103.51	112.60
1	A	212	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	202	ILE	CA-C-O	-5.33	114.89	120.27
1	C	24	GLN	CB-CA-C	-5.33	102.52	110.88
1	C	389	ASN	CA-C-N	-5.32	116.17	123.14
1	C	389	ASN	C-N-CA	-5.32	116.17	123.14
1	A	49	ILE	CA-C-O	-5.32	116.25	121.67
1	C	57	SER	CB-CA-C	5.32	117.66	110.37
1	C	142	HIS	CA-CB-CG	-5.32	108.48	113.80
1	C	75	HIS	CA-CB-CG	-5.31	108.49	113.80
1	C	336	SER	CA-C-O	-5.30	115.56	121.81
1	A	484	TYR	CA-C-N	5.27	129.22	120.94
1	A	484	TYR	C-N-CA	5.27	129.22	120.94
1	A	38	ASN	CA-C-O	-5.26	115.28	121.07
1	C	181	GLN	CA-C-N	5.25	125.30	119.32
1	C	181	GLN	C-N-CA	5.25	125.30	119.32
1	C	187	THR	CA-C-O	-5.24	115.31	121.44
1	A	470	GLU	CA-C-O	5.23	126.10	120.55
1	C	216	THR	CA-C-N	-5.23	117.80	123.08
1	C	216	THR	C-N-CA	-5.23	117.80	123.08
1	C	275	TYR	CA-CB-CG	-5.23	104.49	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	404	ARG	CB-CA-C	5.22	119.46	110.79
1	C	471	GLN	CA-C-O	5.19	126.05	120.55
1	A	485	TYR	O-C-N	5.19	128.98	122.86
1	A	393	GLU	CB-CA-C	5.18	118.72	109.65
1	C	267	ASP	CA-C-N	5.17	125.17	119.90
1	C	267	ASP	C-N-CA	5.17	125.17	119.90
1	A	260	ILE	CA-C-N	5.17	125.47	119.47
1	A	260	ILE	C-N-CA	5.17	125.47	119.47
1	C	251	GLU	N-CA-C	5.16	117.57	111.33
1	C	260	ILE	CA-C-N	5.15	124.65	119.19
1	C	260	ILE	C-N-CA	5.15	124.65	119.19
1	C	161	HIS	N-CA-CB	-5.15	103.09	110.04
1	C	246	ASN	CA-C-N	5.14	130.02	122.77
1	C	246	ASN	C-N-CA	5.14	130.02	122.77
1	C	473	LEU	N-CA-CB	-5.13	102.58	110.12
1	A	395	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	A	181	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	C	86	THR	CA-C-O	5.12	125.91	120.64
1	C	195	ASN	CA-C-O	-5.11	114.47	120.60
1	A	77	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A	179	TRP	CA-CB-CG	5.11	123.30	113.60
1	A	309	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	A	228	SER	O-C-N	-5.08	116.56	122.96
1	A	110	ALA	O-C-N	-5.07	116.74	122.12
1	C	163[A]	SER	O-C-N	5.07	128.98	122.39
1	C	163[B]	SER	O-C-N	5.07	128.98	122.39
1	C	388	VAL	N-CA-CB	-5.07	101.62	110.49
1	A	257	LYS	CA-C-O	5.04	125.78	119.59
1	A	27	ASP	CA-C-N	5.03	124.69	119.56
1	A	27	ASP	C-N-CA	5.03	124.69	119.56
1	A	355	ALA	CA-C-O	-5.02	116.05	121.87
1	A	421	ASN	N-CA-C	5.01	117.40	107.98
1	C	49	ILE	CA-C-O	-5.00	116.57	121.67
1	A	2	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4171	0	4084	56	0
1	C	4173	0	4084	22	0
2	B	23	0	31	0	0
2	D	23	0	31	2	0
3	C	1	0	0	0	0
4	A	124	0	0	1	0
4	B	3	0	0	0	0
4	C	209	0	0	2	0
4	D	3	0	0	0	0
All	All	8730	0	8230	78	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (78) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LYS:HD2	1:A:68:ASP:OD2	1.97	0.65
1:A:117:HIS:NE2	1:A:454:LEU:HD11	2.13	0.63
1:A:229:GLU:O	1:A:233:VAL:HG23	1.99	0.62
1:A:43:LEU:HD21	1:A:204:LEU:HD22	1.81	0.62
1:C:390:VAL:HG13	4:C:714:HOH:O	1.99	0.61
1:A:229:GLU:HB3	1:A:249:PRO:HD3	1.79	0.61
1:A:236:TYR:O	1:A:492:LYS:NZ	2.34	0.61
1:A:4:PRO:HD2	1:A:7:VAL:HG21	1.83	0.61
1:C:459:ASP:OD1	1:C:462:ARG:NH1	2.32	0.61
1:C:346:LYS:NZ	1:C:350:GLU:OE2	2.33	0.61
1:C:218:ILE:HD11	1:C:514:ILE:HG12	1.83	0.59
1:C:253:PHE:CE2	1:C:257:LYS:HD2	2.38	0.59
1:A:355:ALA:O	1:A:356:ASP:HB3	2.02	0.58
1:A:377:ALA:O	1:A:381:ILE:HG13	2.05	0.57
1:A:260:ILE:HD12	1:A:263:GLU:HB2	1.85	0.57
1:A:113:LEU:HD22	1:A:118:ILE:HD12	1.86	0.57
1:C:21[A]:SER:HB3	4:C:672:HOH:O	2.04	0.56
1:A:24:GLN:HA	1:A:398:LYS:HE3	1.88	0.55
1:A:365:TYR:OH	1:A:372:LYS:HD3	2.05	0.55
1:A:24:GLN:HG3	1:A:36:GLU:OE2	2.06	0.54
1:A:255:LYS:HD2	1:A:259:GLU:OE1	2.10	0.51
1:A:323:ASP:HB2	1:A:421:ASN:OD1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:VAL:HG11	1:A:252:LEU:HD12	1.93	0.51
1:C:302:ILE:HD11	1:C:381:ILE:HD12	1.91	0.51
1:A:3:VAL:HG11	1:A:9:LEU:HD21	1.93	0.50
1:A:4:PRO:O	1:A:7:VAL:HG23	2.11	0.50
1:A:257:LYS:O	1:A:257:LYS:HG3	2.09	0.49
1:A:301:ILE:HA	1:A:305:LYS:HD2	1.93	0.49
1:A:357:LYS:N	1:A:358:PRO:HD3	2.28	0.49
1:C:359:LEU:HB3	1:C:388:VAL:HG22	1.94	0.49
1:A:307:LYS:HD3	1:A:311:ASP:OD2	2.13	0.48
1:C:115:TYR:CE1	1:C:428:ASN:HB3	2.48	0.48
1:A:19:ASN:N	1:A:224:LEU:O	2.40	0.48
1:C:398:LYS:HB3	1:C:398:LYS:NZ	2.29	0.48
1:A:448:LYS:HD3	1:A:452:ASP:OD2	2.14	0.48
1:A:402:ASP:OD2	1:A:406:GLN:NE2	2.47	0.47
1:C:398:LYS:HG3	1:C:399:THR:N	2.28	0.47
1:C:137:LYS:HE2	1:C:145:GLU:OE1	2.14	0.47
1:C:218:ILE:CD1	1:C:514:ILE:HG12	2.44	0.47
1:A:161:HIS:CD2	1:A:162:PRO:HD2	2.50	0.47
1:A:63:LYS:HD3	1:A:64:TRP:N	2.30	0.47
1:A:307:LYS:HE2	1:A:370:LEU:HD11	1.97	0.47
1:A:265:ARG:NH2	1:A:498:TYR:O	2.49	0.46
1:C:398:LYS:HB3	1:C:398:LYS:HZ2	1.81	0.46
1:C:269:TYR:HE2	2:D:3:LYS:HE3	1.80	0.46
1:C:113:LEU:HD22	1:C:118:ILE:HD12	1.97	0.45
1:A:366:ASN:O	1:A:367:THR:C	2.59	0.45
1:C:210:TYR:CE2	1:C:212:ASP:HB3	2.52	0.45
1:A:360:THR:HA	1:A:389:ASN:O	2.16	0.45
1:A:453:THR:O	1:A:462:ARG:HD3	2.18	0.44
1:C:260:ILE:O	1:C:260:ILE:HG13	2.17	0.44
1:A:355:ALA:O	1:A:356:ASP:CB	2.64	0.43
1:A:84:ASP:OD1	1:A:86:THR:HG23	2.18	0.43
1:A:117:HIS:CD2	1:A:454:LEU:HD11	2.54	0.43
1:A:236:TYR:O	1:A:237:ARG:C	2.62	0.43
1:A:248:MET:HA	1:A:248:MET:HE2	2.00	0.43
1:A:359:LEU:HB3	1:A:388:VAL:HG12	2.01	0.42
1:A:10:ALA:HA	1:A:516:LYS:HG3	2.01	0.42
1:A:362:ASP:OD1	1:A:391:ASN:HB2	2.20	0.42
1:A:312:LEU:HD22	1:A:312:LEU:N	2.35	0.42
1:A:43:LEU:O	1:A:187:THR:HB	2.20	0.42
1:A:365:TYR:CZ	1:A:394:ASN:HB3	2.54	0.42
1:A:329:GLU:OE1	1:A:334:LYS:NZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:VAL:O	1:A:199:ASN:HB2	2.19	0.42
1:C:269:TYR:OH	2:D:3:LYS:HE2	2.19	0.42
1:A:16:VAL:CG1	1:A:224:LEU:HD11	2.50	0.41
1:A:267:ASP:HB3	1:A:268:PRO:CD	2.50	0.41
1:A:3:VAL:HA	1:A:4:PRO:HD3	1.75	0.41
1:A:180:THR:HA	1:A:185:ILE:HD12	2.02	0.41
1:A:269:TYR:HB2	1:A:487:ASN:HB2	2.00	0.41
1:C:150:GLU:HB3	1:C:151:PRO:HD2	2.01	0.41
1:A:267:ASP:HB3	1:A:268:PRO:HD2	2.03	0.41
1:A:209:GLN:HA	1:A:209:GLN:HE21	1.85	0.41
1:A:357:LYS:N	1:A:358:PRO:CD	2.84	0.41
1:A:341:ASN:O	1:A:345:LYS:HE3	2.21	0.41
1:A:516:LYS:HA	4:A:633:HOH:O	2.21	0.41
1:C:258:LYS:HE3	1:C:258:LYS:HB2	1.78	0.40
1:C:402:ASP:OD2	1:C:406:GLN:NE2	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	517/517 (100%)	488 (94%)	27 (5%)	2 (0%)	30	27
1	C	519/517 (100%)	509 (98%)	9 (2%)	1 (0%)	43	42
2	B	1/3 (33%)	1 (100%)	0	0	100	100
2	D	1/3 (33%)	1 (100%)	0	0	100	100
All	All	1038/1040 (100%)	999 (96%)	36 (4%)	3 (0%)	36	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	PRO
1	A	51	ASP
1	C	225	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	457/455 (100%)	424 (93%)	33 (7%)	13	10
1	C	459/455 (101%)	437 (95%)	22 (5%)	23	21
2	B	2/2 (100%)	2 (100%)	0	100	100
2	D	2/2 (100%)	2 (100%)	0	100	100
All	All	920/914 (101%)	865 (94%)	55 (6%)	17	14

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	21	SER
1	A	52	VAL
1	A	63	LYS
1	A	65	GLU
1	A	67	LYS
1	A	78	GLU
1	A	137	LYS
1	A	181	GLN
1	A	209	GLN
1	A	221	VAL
1	A	230	VAL
1	A	237	ARG
1	A	252	LEU
1	A	255	LYS
1	A	256	LEU
1	A	257	LYS
1	A	300	ASP
1	A	312	LEU

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Mol	Chain	Res	Type
1	A	323	ASP
1	A	326	LYS
1	A	342	GLU
1	A	357	LYS
1	A	372	LYS
1	A	381	ILE
1	A	384	LYS
1	A	390	VAL
1	A	396	GLU
1	A	413	ARG
1	A	431	LEU
1	A	460	THR
1	A	510	LYS
1	A	515	ILE
1	C	11	ASP
1	C	58	PRO
1	C	65	GLU
1	C	209	GLN
1	C	255	LYS
1	C	283	PRO
1	C	312	LEU
1	C	326	LYS
1	C	338	GLN
1	C	345	LYS
1	C	348	LEU
1	C	384	LYS
1	C	388	VAL
1	C	390	VAL
1	C	393	GLU
1	C	398	LYS
1	C	413	ARG
1	C	431	LEU
1	C	454	LEU
1	C	473	LEU
1	C	475	LYS
1	C	516	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	104	ASN

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Mol	Chain	Res	Type
1	A	181	GLN
1	A	199	ASN
1	A	207	ASN
1	A	209	GLN
1	A	220	GLN
1	A	391	ASN
1	A	406	GLN
1	A	461	GLN
1	C	104	ASN
1	C	199	ASN
1	C	338	GLN
1	C	395	GLN
1	C	461	GLN
1	C	471	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.